

# CROATICA CHEMICA ACTA

---

*Croat. Chem. Acta* Vol. **74** No. 2

207–477, A39–A40, C7–C8 (2001)

Zagreb, April, 2001

---

## CONTENTS

### Proceedings of the Fifteenth Dubrovnik International Course and Conference MATH/CHEM/COMP 2000 and of the Third International Dubrovnik NMR Course and Conference DU 2000 NMR

Foreword	. . . Ante Graovac and Dražen Vikić-Topić	I–II
Same Time Next Year in Dubrovnik, Croatia (Poem)	. . . Frank Harary	III

#### *Graph Theory and Topological Indices*

Two Models for Random Graphs with Bounded Degree . . . Krystyna T. Balińska, Michael L. Gargano, and Louis V. Quintas	207–223
Randić Index of Benzenoid Systems and Phenylenes . . . Juan Rada, Oswaldo Araujo, and Ivan Gutman	225–235
Predicting Inhibition of Microsomal <i>p</i> -Hydroxylation of Aniline by Aliphatic Alcohols: A QSAR Approach Based on the Weighted Path Numbers . . . Dragan Amić, Bono Lučić, Sonja Nikolić, and Nenad Trinajstić	237–250

#### *Theoretical and Computational Chemistry*

Mechanism of Gas Phase Ethene-Ozone Reaction and Concomitant Processes. Theoretical Study . . . Robert Ponec, Jana Roithová, and Yehuda Haas	251–264
<i>Ab initio</i> Theoretical Investigation of a Formal Alkene-Enedione Intramolecular [2 + 2] Photocyclization . . . Alan P. Marchand, Trevor D. Power, and Hendrik G. Kruger	265–270
On the Proton Affinity of Peroxynitrite and Peroxynitrous Acid . . . Saša Kazazić, Snježana Kazazić, Leo Klasinc, Sean P. McGlynn, and William A. Pryor	271–275
Computational Studies of Chemical Shifts Using Density Functional Optimized Geometries. II. Isotropic <sup>1</sup> H and <sup>13</sup> C Chemical Shifts and Substituent Effects on <sup>13</sup> C Shieldings in 2-Adamantanone . . . Dražen Vikić-Topić and Ljupčo Pejov	277–293

*(Continued on inside back cover)*

(Continued from outside back cover)

- COMBINE Analysis of Nuclear Receptor-DNA Binding Specificity: Comparison of Two Sets of Data . . . **Sanja Tomić and Rebecca C. Wade** 295–314
- A Sensitivity Model and Repeatability of Recipe Colour . . . **Boris Sluban and Olivera Šauperl** 315–325

*Modelling in Chemistry and Biochemistry*

- Conformational Behaviour of 11-*O*-Methylazithromycin in the Solid and Solution State . . . **Nada Košutić-Hulita, Dijana Matak-Vinković, Mladen Vinković, Predrag Novak, Gabrijela Kobrehel, and Gorjana Lazarevski** 327–341
- Enantioselectivity of *Pseudomonas cepacia* Lipase towards 2-Methyl-3(or 4)-aryl-alkanols: An Approach Based on the Stereoelectronic Theory and Molecular Modeling . . . **Sanja Tomić, Vladimir Dobovičnik, Vitomir Šunjić, and Biserka Kojić-Prodić** 343–357

*Synthesis and Spectroscopy*

- Preparation, Thermal Analysis and Spectral Characterization of the 1:1 Complexes of Mercury(II) Halides and Pseudohalides with 3,4,5,6-Tetrahydropyrimidine-2-thione. Crystal Structures of Bis(3,4,5,6-tetrahydropyrimidine-2-thione-S)mercury(II) Tetrachloro and Tetrabromomercurate(II) . . . **Zora Popović, Dubravka Matković-Čalogović, Gordana Pavlović, Željka Soldin, Gerald Giester, Maša Rajić, and Dražen Vikić-Topić** 359–380
- NMR Conformational Study Reveals that S-C-N Anomeric Effect in Thionucleosides Is Weaker than O-C-N Anomeric Effect in Natural Nucleosides . . . **Martin Črnugelj and Janez Plavec** 381–398
- Synthesis, NMR and MS Study of Novel *N*-Sulfonylated Purine Derivatives . . . **Biserka Žinić, Irena Krizmanić, Dražen Vikić-Topić, Dunja Srzić, and Mladen Žinić** 399–414

**Regular Scientific Papers**

*Inorganic Chemistry*

- An Improved Synthesis of Tetramethylammonium Azide . . . **Dirk Schweitzer** 415–418

*Materials Chemistry*

- Influence of X-ray Radiation on the Phase Composition and Morphology of Electric Furnace Slag, Clinker, and Plaster . . . **Alenka Rastovčan-Mioč, Štefica Cerjan-Stefanović, Vjera Novosel-Radović, Boro Mioč, and Tahir Sofilić** 419–430



(Continued on the preceding page)

(Continued from inside back cover)

*Organic Chemistry*

Composition of Free and Glycosidically Bound Volatiles of *Mentha aquatica* L.  
... **Igor Jerković and Josip Mastelić** 431–439

Synthesis and Structure of Two Isomeric Enaminones  
... **Ana Brbot-Šaranović, Gordana Pavlović, Višnja Vrdoljak,  
and Marina Cindrić** 441–454

*Biochemistry*

Substituted Guanidine Compounds as Inhibitors of Nonenzymatic Glycation *in vitro*  
... **Irena Mišur and Zdenka Turk** 455–465

*Analytical Chemistry*

Extraction and Separation of Germanium(IV) with 4-Pyridone Derivatives  
... **Vlasta Vojković, Iva Juranović, and Biserka Tamhina** 467–477

Erratum A39

Book Review A40

Announcements and Advertisements C7–C8